Materials for Transduction (MATRIX)

Proposers Day

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MATRIX Proposer's Day Workshop
Arlington, VA

January 23, 2015

MATRIX Agenda

- MATRIX Program Motivation and Overview
- MATRIX Program Objectives
- MATRIX Program Challenges and Applications
- Proposal Guidance

Disclaimer:

In the event of a disagreement between the contents of the BAA and the information in this briefing, please follow the BAA. No exceptions.

MATRIX Vision: New classes of transductional materials and devices

Problem

DARPA/DoD achievements in engineered transductional materials have not transitioned to new DoD capabilities

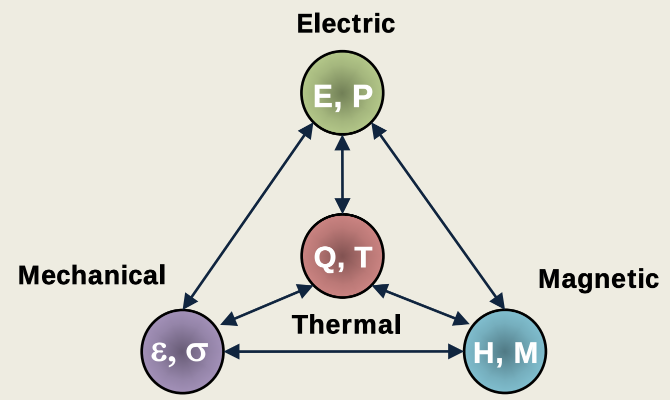
Goal

Extend material breakthroughs to the device and system level

MATRIX Approach

Integrate transduction modeling, design and validation into unified R&D approach with applications focus

Energy Transduction Diagram



Example Transductional Materials

- **Thermoelectrics** – energy harvesting, thermal management, refrigeration
- **Multiferroics** – sensors, micromotors and transducers, tunable RF components
- **Phase Change Materials** – transducers, switches, control and logic devices

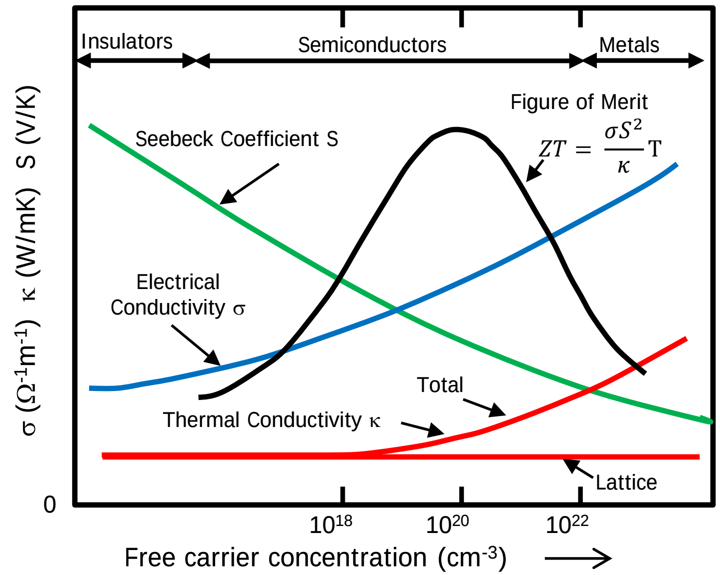
MATRIX aims to bridge the gap between transductional material breakthroughs and new DoD capabilities

Thermoelectrics case example: promise and challenges

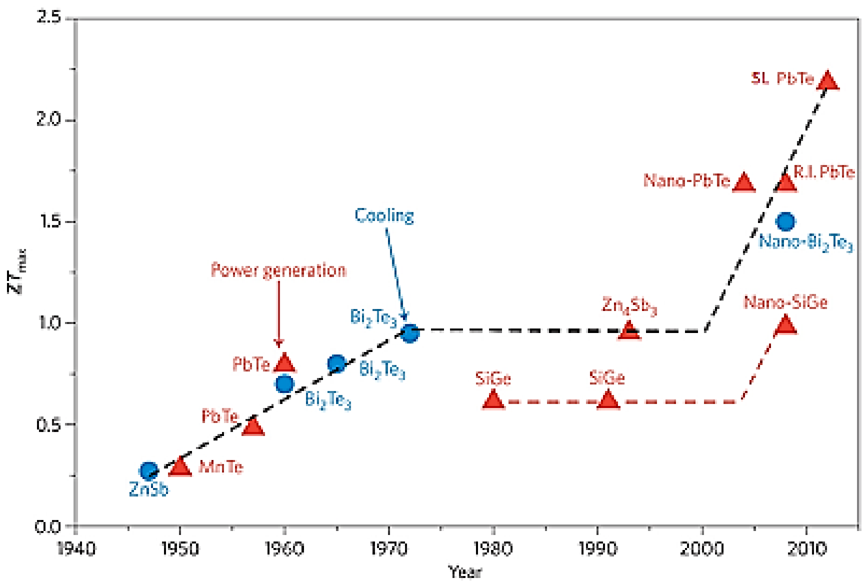
Thermoelectric Challenge

- Requires contradictory material properties
  - High Seebeck coefficient -> semiconductors
  - High electrical conductivity -> metals
  - Low thermal conductivity - > insulators

ZT Figure of Merit



ZT progress in materials



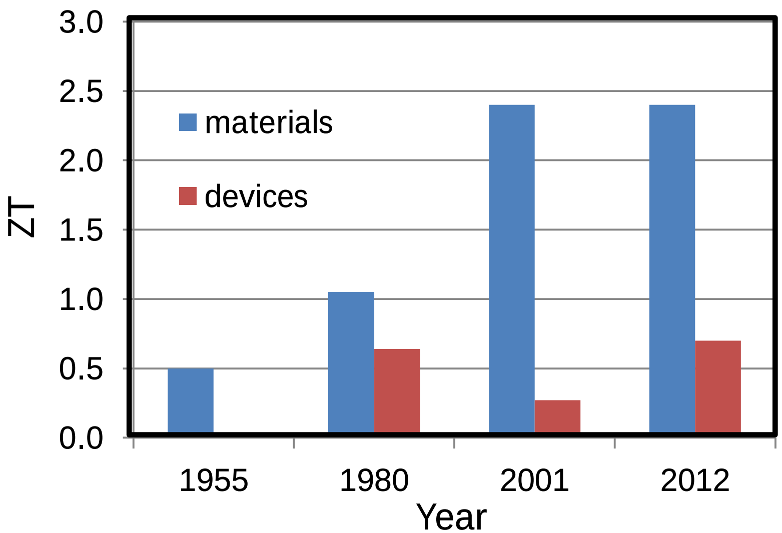
Recent achievements

- Progress in p- and n-type materials in last decade breaks ZT > 1 barrier
- $ZT_{material}$ > 2 for some materials at T_{max}
- However, different materials don't achieve max ZT at the same temp
- Effective device ZT's remain < 1

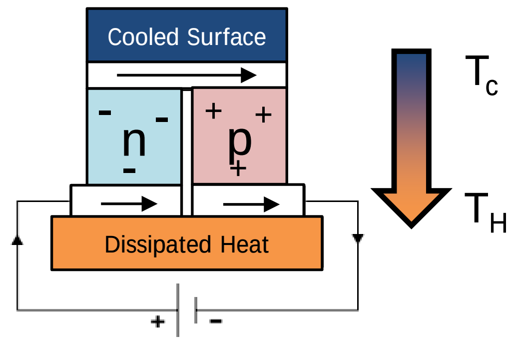
Advances in thermoelectric materials, *but* ...

Thermoelectrics materials and devices

ZT for ambient temperature TE materials & devices



TE Device

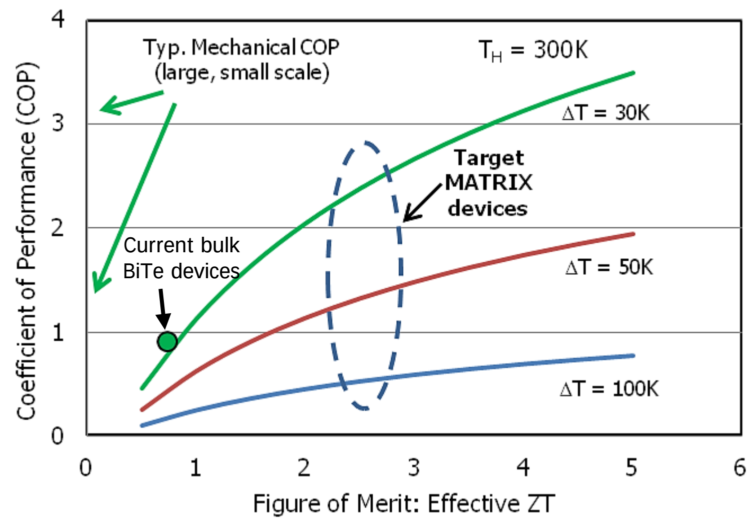


- Progress at materials level has not translated to device COP
  - Unbalanced n- and p- type material paths
  - Suboptimal electrical and thermal contacts
  - Suboptimal performance at operating temp and across ΔT

⇨ Effective $ZT_{device} < 1$

ZT and COP

$$COP_{max} \approx \left(\frac{T_C}{T_H - T_C}\right)\left(\frac{\sqrt{1+ZT_{av}} - \frac{T_H}{T_C}}{\sqrt{1+ZT_{av}}+1}\right)$$



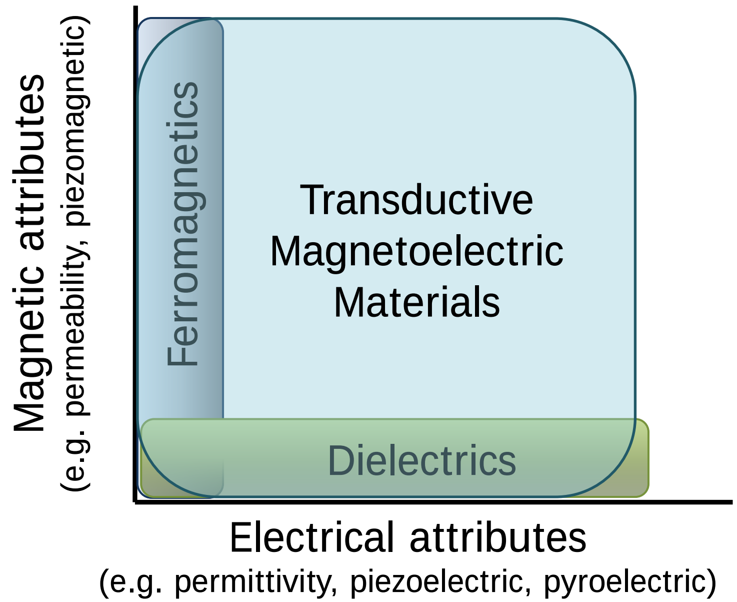
Advances in materials have not led to device gains: we need an integrated approach – "The material is the device"

Multiferroics Challenges

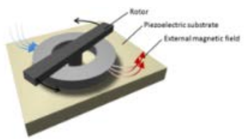
- Overcome contradictory fusion of materials properties and parameters
  - E.g. high permeability, piezoelectricity, piezomagnetism
- Highly efficient energy transduction, high Q, low loss

	Multiferroic Materials*	Coupling Constant A (Oe cm / kV)
Measured	YIG	10^{-10}
Measured	$Fe_xGa_{2-x}O_3$	10^{-6}
Measured	Nickel ferrite-PZT	0.7
Measured	YIG-PZT	1
Measured	LFO-PZT	10
Measured	NFO-PZT	20
Measured	Ni-PZT	50
Modeled	YIG-PMN-PT	~50
Modeled	LFO-PMN-PT	~200
Modeled	FeGaB-PZN-PT	~300

Increased Energy Coupling



Multiferroics application examples



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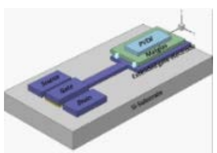
- High magnetic field density (~Tesla) without high current density -> new generation of micro motor and actuator applications



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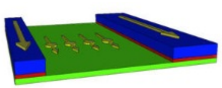
- Transduction of energy allows for high sensitivity room temp sensors, antennas at low Size, Weight and Power (SWaP)



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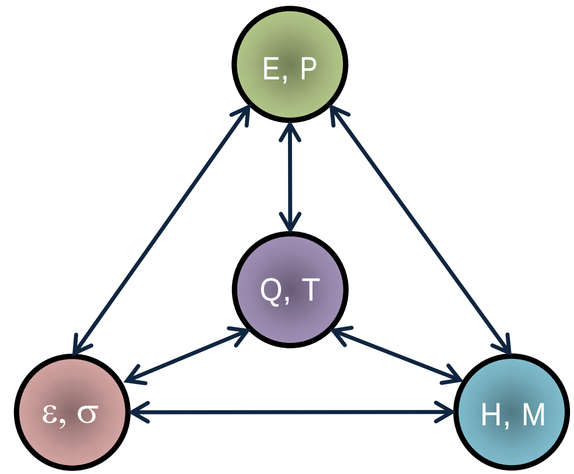
- Precise control and tunability of properties (permittivity, permeability, E and B fields) -> new tunable filters, inductors, circulators, transformers, EM spectral control



Lattice strain (elastic/acoustic modes) couples electric and magnetic field modes

* Source: Internet

System approach – what's new

Bridge between transductional materials science and predictive models

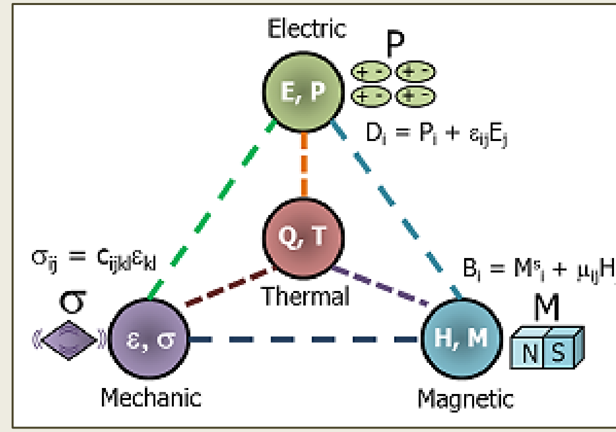
- Integrated multi-modal modeling of lattice, carrier, and order dynamics
  - Understanding of resonances, efficiency and loss
  - Dynamic coupled modalities
- Extend first principles modeling with new models that capture new materials structures of interest

Rapid experimental validation of models

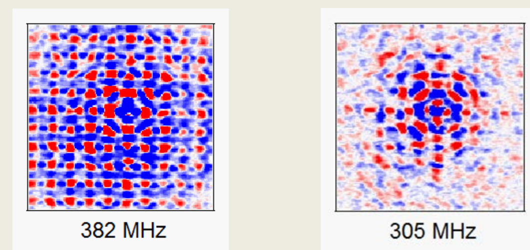
- New experimental tools; rapid validation of phonon dynamics modeling

System-level architecture & optimization

- Integrated materials, device, systems communities
- Coupled materials, device and systems models
- System focus on multiscale, transductional materials/devices

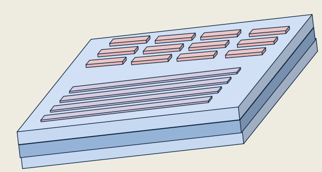


Transductance often mediated by non-direct ordering; eg: strain-mediated magnetoelectric



Phonon propagation in bulk material　　*Phonon propagation with engineered bandgap*

Hokkaido University Laboratory of Applied Solid State Physics



"The material is the device"

MATRIX program elements

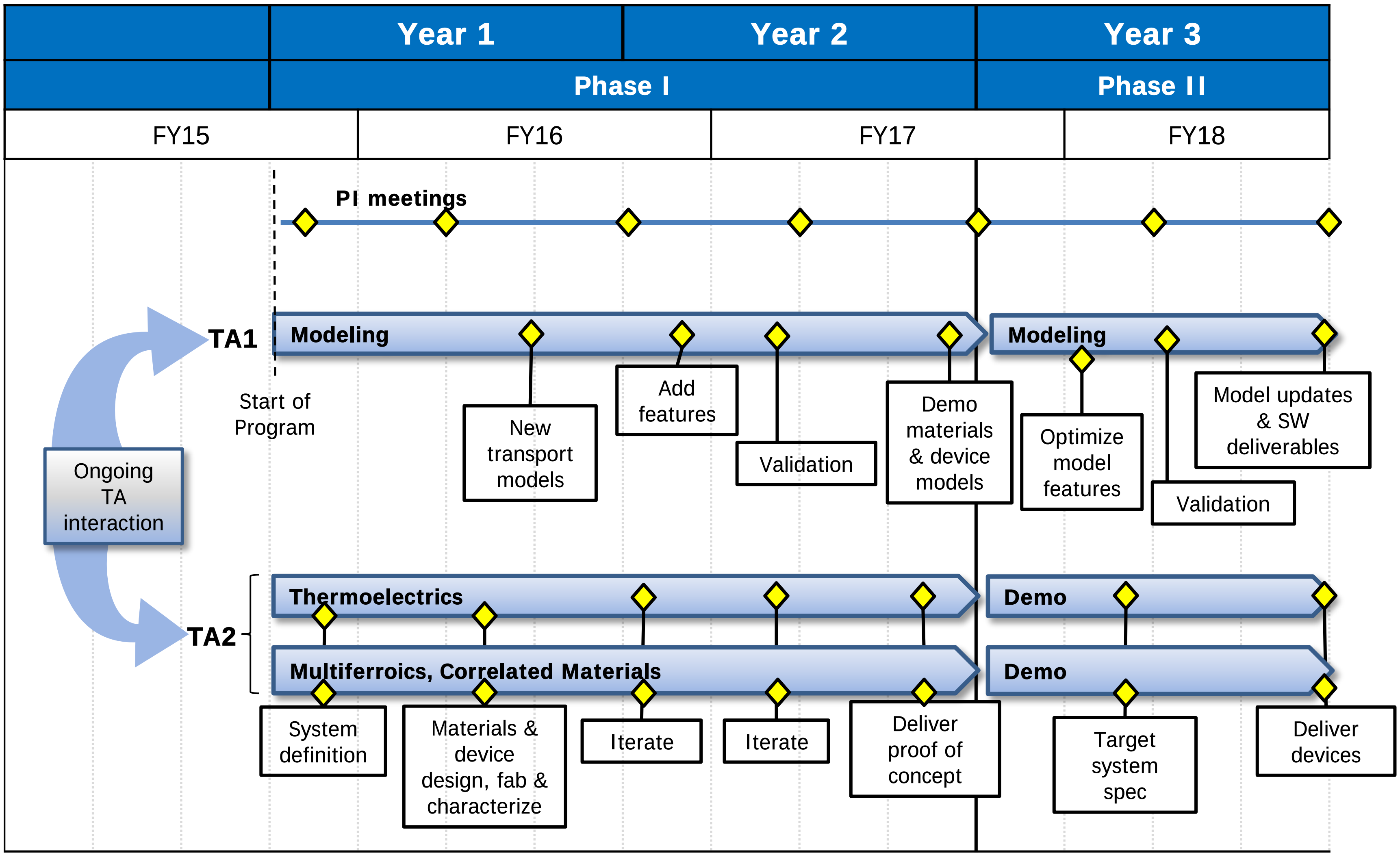
Technical Area 1: Transduction Modeling

- Ab initio models addressing carrier transport, complex engineered materials structures, strong correlations
- Carrier transport metrology and model validation (optional)
- TA1 runs in parallel to TA2 and is tightly coupled

Technical Area 2: Thermoelectrics (TA2a) Multiferroics & Correlated Materials (TA2b)

- Application focus
- Systems-level architecture and optimization
- Integrated multimodal transduction engineering models
- Integrated materials & device development

MATRIX notional timeline



Proposal Guidance

For TA1 proposals:

- Summarize the materials/device structures to be modeled
- Summarize theoretical and modeling approach
- Summarize key innovations, how your approach advances beyond current practice
- Key expected outputs and deliverables
- Plan for experimental validation (if part of proposal)

For TA2 proposals:

- Summarize application and device to be demonstrated
- Summarize technical approach (materials and device structure)
- Summarize key innovations, how your approach advances beyond current practice
- Key expected outputs and deliverables

Modeling and Computational Tools (TA1 Only)

Modeling and Computational Tools Table (TA1)		
Modeling Method		
Devices Impacted		
Materials structure		
Deficiencies Addressed	**SOA**	**Improvement**
e.g. better correlation of first principles predictions with experimental results		
e.g. more accurate prediction of Seebeck coefficient and thermal conductivity for a family of engineered materials		

Application, Metrics and Specifications (TA2 Only)

Application and Device Table (TA2)				
Application				
Device				
Materials structure				
Metrics	**SOA**	**Proposed New**	**Verification Metrology**	**Key Risk & Mitigation**
Key Materials Metrics				
e.g. electrical & thermal conductivity				
e.g. Seebeck coef				
e.g. ZT at T1, T2				
Key Device Metrics				
Operating temperature				
e.g. COP at DeltaT				
SWaP				

More proposal guidance

Read the BAA! (If the BAA differs from this presentation, be guided by the BAA)

For TA2:

- Present a compelling, DoD-relevant application that can't be addressed by current SOA
- Present a novel and innovative approach at both materials and device levels
- Back up your idea and technical approach (e.g. by theoretical arguments, models, past results, new data)
- Address all of the technology axes of relevance to the application
- Provide quantitative metrics for both the materials and the device

For TA1:

- Tell us how you are going to advance the science of transductional materials, what classes of new materials will be addressed, and how the work will impact the community of transductional materials and device engineers